

Aldicarb
116-06-3 | DTXSID0039223

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 253 °C

Global applicability domain: Inside

Local applicability domain index: 2.70e-01

Confidence level: 6.15e-01

Nearest Neighbors from the Training Set

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Carbamic acid, phenyl-, ethyl ester

Measured: 238

Predicted: 260

[Image not found](#)

Ethyl benzylcarbamate

Measured: 230

Predicted: 255

[Image not found](#)

1,3-Dipropylurea

Measured: 255

Predicted: 256

[Image not found](#)

N,N',N'-Trimethylurea

Measured: 233

Predicted: 233

[Image not found](#)

2-Nitrobenzamide

Measured: 317

Predicted: 310